# Isophthalic acid, 4-chloro-3-methylphenyl pentyl ester

**Inchi:** InChI=1S/C20H21ClO4/c1-3-4-5-11-24-19(22)15-7-6-8-16(13-15)20(23)25-17-9-10-18(21

**InchiKey:** UTFKHQRZPUTQDH-UHFFFAOYSA-N

**Formula:** C20H21ClO4

**SMILES:** CCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1

**Mol. weight [g/mol]:** 360.83

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -166.32 | kJ/mol | Joback Method |
| hf | -522.82 | kJ/mol | Joback Method |
| hfus | 44.24 | kJ/mol | Joback Method |
| hvap | 89.35 | kJ/mol | Joback Method |
| log10ws | -6.64 | | Crippen Method |
| logp | 5.215 | | Crippen Method |
| mcvol | 272.260 | ml/mol | McGowan Method |
| pc | 1644.42 | kPa | Joback Method |
| rinpol | 2895.00 | | NIST Webbook |
| rinpol | 2895.00 | | NIST Webbook |
| tb | 915.31 | K | Joback Method |
| tc | 1144.16 | K | Joback Method |
| tf | 579.80 | K | Joback Method |
| vc | 1.036 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 802.07 | J/mol×K | 915.31 | Joback Method |
| cpg | 852.38 | J/mol×K | 1106.02 | Joback Method |
| cpg | 844.79 | J/mol×K | 1067.88 | Joback Method |
| cpg | 836.00 | J/mol×K | 1029.74 | Joback Method |
| cpg | 825.96 | J/mol×K | 991.59 | Joback Method |
| cpg | 814.66 | J/mol×K | 953.45 | Joback Method |
| cpg | 858.78 | J/mol×K | 1144.16 | Joback Method |
| dvisc | 0.0000505 | Pa×s | 915.31 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000625 | Pa×s | 859.39 | Joback Method |
| dvisc | 0.0000798 | Pa×s | 803.47 | Joback Method |
| dvisc | 0.0001057 | Pa×s | 747.56 | Joback Method |
| dvisc | 0.0001464 | Pa×s | 691.64 | Joback Method |
| dvisc | 0.0002149 | Pa×s | 635.72 | Joback Method |
| dvisc | 0.0003394 | Pa×s | 579.80 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344592&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |